

Application of a Hydrobiogeochemistry Computer Model to Fate and Transport of Co-contaminants in Fractured Saprolite

We have developed a hydrobiogeochemistry model HBGC123D (HydroBioGeoChemistry in 1, 2, and 3 Dimensions). The program is capable of simulating solute and heat transport and a wide range of coupled reactions. Both equilibrium and kinetic geochemical and microbial reactions can be simulated. The software and its documentation are freely available on the WWW at <http://hbgc.esd.ornl.gov>.

The Oak Ridge Reservation (ORR) in Oak Ridge, TN is one of several U.S. Department of Energy facilities where large quantities of low-level radioactive waste have been stored underground in previous decades. This waste comprises organically complexed contaminants (co-contaminants) like CoEDTA and CdEDTA. While it was assumed at the time of the waste deposition that co-contaminants are immobile due to adsorption, investigations on the ORR have shown that co-contaminants may be transported into the groundwater. In order to improve our understanding of the transport behavior of co-contaminants on the field-scale, several laboratory experiments were conducted. These experiments were performed on undisturbed soil columns obtained from the ORR. The soil consists primarily of highly fractured saprolite.

HBGC123D was applied to simulate the transport and reactions of CoEDTA and CdEDTA in two of these columns. In the first experiment, CdEDTA²⁻ was injected and adsorbed to iron oxides in the solid phase. The adsorption of the CdEDTA²⁻ ligand resulted in the formation and release of Fe(III)EDTA⁻ and Cd²⁺. In the second experiment, Co(II)EDTA²⁻ was injected and oxidized to Co(III)EDTA⁻ with amorphous Mn(IV) oxides as the oxidizing agent. Aqueous manganese (Mn²⁺) was released from the solid phase and measured in the effluent. Bromide was used in both experiments as a non-reactive tracer. This enabled us to determine the dispersion coefficient. The simulations included the most important reactions, i.e. adsorption, complexation, precipitation and redox reactions. The complexity of the system resulted in a large number of reaction parameters that had to be determined, mostly the kinetic rate coefficients. Our simulation results are in fairly good agreement with the measured breakthrough curves. The parameters determined from the column simulations are being used to investigate coupled hydrological and geochemical processes at a field site at ORR where co-contaminants were released and monitored.